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# Diffusive-ballistic heat transport in thin films using energy conserving dissipative particle dynamics

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ABSTRACT

Diffusive-ballistic heat transport in thin films was simulated using energy conserving dissipative particle dynamics (DPDe). The solution domain was considered to be two-dimensional with DPD particles distributed uniformly under constant temperature boundary conditions at the top and bottom walls and periodic boundaries at the side walls. The effects of phonon mean free path were incorporated by its relation to the cutoff radius of energy interaction. This cutoff radius was based on the Knudsen number using the existing phonon-boundary scattering models. The simulations for $0.1 < Kn < 10$ were obtained with the different modifications of the cutoff radius. The results were presented in form of a nondimensional temperature profile across the thin film and were compared with the semi-analytical solution of the equation of phonon radiative transport (EPRT). When the phonon-boundary scattering is not considered, the DPDe simulation results have more discrepancies compared with the EPRT solution as *Kn* increases, indicating that the phonon-boundary scattering plays an important role when the heat transport across the film becomes more ballistic. The results demonstrate that the DPDe can simulate the diffusive-ballistic heat transport for a broad range of *Kn*, but phonon-boundary scattering should be considered for the accurate simulation of the ballistic heat transport.



## 1. Introduction

Micro/nano structures, such as thin films, nanotubes and nanowires, have been widely utilized for a number of electronics, micro- and nano- electromechanical systems (MEMS and NEMS) and molecular-scale microscopic devices [1]. The size of these structures are in the order of less than a micrometer. In such small scales, the heat transport is quite different from the macro-scale continuum assumption (e.g., Fourier's law) due to the small characteristic length that is comparable to or smaller than the mean free path of the energy carriers. Therefore, it is imperative to understand the detailed phenomena of heat transfer at micro/nano scale for the further development of these devices.

For dielectric materials and semiconductors, the heat transfer is dominated by lattice vibration. The quanta of the vibration energy are called phonons. Phonon-based heat transport is crucially important when the phonon mean free path becomes comparable to the characteristic length of the micro/nano structures. Joshi and Majumdar [2] derived the equation of phonon radiative transfer (EPRT) from the Boltzmann transport equation (BTE) to study the heat transport in diamond thin films of different film thicknesses. The EPRT was numerically solved using the explicit upstream differencing method. The results showed that the heat transport in thin films is not purely diffusive and becomes partially ballistic when the thickness becomes comparable to the phonon mean free path. Chen [3,4] modified the BTE with the gray relaxation time approximation and derived the ballistic-diffusive equation by dividing the phonon distribution function (or the phonon intensity) into ballistic and diffusive parts. This ballistic-diffusive approximation is much simpler than BTE. However, the results showed that this model is not accurate when the diffusive heat transport is dominant, i.e., the phonon mean free path is smaller than the film thickness.

In addition to these studies, other analytical [1,5] and numerical investigations [6–11] showed similar trends in nanotubes and nanowires. However, most analyticial studies to date have been limited to simple one-dimensional nanostructures, such as thin films and wires, to be tractable to analytical and numerical solutions and physical interpretation. For most numerical studies, molecular dynamics (MD) has been employed since it is flexible in terms of the degree of freedom for computation domain and in dealing with geometrical complexities. However, MD is an extremely expensive numerical simulation and hence can hardly be applied for simulations at meso- or macroscales. For this reason,

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a new method needs to be developed which captures both the applicability to multi-scale domains and requires relatively reasonable computational cost.

Dissipative particle dynamics (DPD) is a relatively new particle-based simulation method introduced by Hoogerbrugge and Koelman [12] and has great potential applications to mesoscopic simulations. It is a coarse-grained version of molecular dynamics in which each DPD particle represents a cluster of actual molecules moving in a Lagrangian fashion [13,14]. DPD was originally applied to isothermal systems. However, an energy conserving DPD (DPDe) method [15,16] was developed for non-isothermal problems by adding the energy conservation equation to the DPD simulation. The DPDe scheme has been utilized for the simulations of various heat conduction, forced convection and natural convection scenarios [17–22]. and the results were in good agreement with analytical and continuum-based numerical solutions. There are also some studies investigating the heat transfer in nano-composites and nanofluids using DPDe [23,24]. However, these models are based on the continuum-based assumption. There has been no previous study to date on heat transport in diffusive-ballistic regimes using DPDe.

The present article demonstrates the application of DPDe for diffusive-ballistic heat transport in thin films. A methodology will be introduced to model the mean free path of phonon by its relation to the cutoff radius of energy interaction. The effect of phonon-boundary scattering is incorporated by employing the existing analytical models. Benchmark simulations are first performed to examine the effects of computational parameters on the numerical results and computational cost. In order to benchmark this method, steady heat transport in one-dimensional thin films is solved over a wide range of Knudsen numbers and the results are compared with the semi-analytical solutions of EPRT.

## 2. Methodology

### 2.1. DPD governing equations

While the detailed description of the DPDe for conduction and convection heat transfer simulations can be found in Ref. [22], its formulation will be briefly reviewed in this section. In the DPD method, each DPD particle interacts with the surrounding particles through a set of distance- and velocity-dependent forces and energies within a certain cutoff radius. In the heat conduction problems, the motion of the DPD particles are not considered, and thus the DPD momentum equation is ignored. For the energy conservation in a DPD system, the following energy equation is used [15,16]:

$$C_v \frac{dT_i}{dt} = q_{ij} \tag{1}$$

where $T_i$ is temperature. $C_v$ is the heat capacity at constant volume of a DPD particle. It is suggested in Ref. [25] that the dimensionless heat capacity, $C_v/k_B$, at meso-scale is $C_v/k_B \gg 1.0$. $q_{ij}$ is the volumetric inter-particle energy interaction rate between DPD particles and consists of three parts as follows:

$$q_{ij} = q_{ij}^V + q_{ij}^C + q_{ij}^R \tag{2}$$

The change in mechanical energy causes viscous heating and is indicated in the form of $q_{ij}^V$, which is ignored in the solid heat conduction because of no motion of the particles. The change in internal energy consists of two terms: one corresponds to the heat transport due to a temperature difference $\left(q_{ij}^C\right)$, and the other takes into account the random heat flux caused by thermal fluctuation $\left(q_{ij}^R\right)$. $q_{ij}^C$, and $q_{ij}^R$ are expressed as [20,21]

$$q_{ij}^C = \sum_{j\neq i} \kappa_{ij}\omega(r_{ij})\left(\frac{1}{T_i} - \frac{1}{T_j}\right) \tag{3}$$

$$q_{ij}^R = \sum_{j\neq i} \alpha_{ij}\omega(r_{ij})^{\frac{1}{2}}\zeta_{ij}^e \Delta t^{-\frac{1}{2}} \tag{4}$$

As shown in these equations, $q_{ij}^C$ is proportional to $\Delta(1/T)$, instead of $\Delta T$, which is related to the irreversible internal nergy interactions between particles in the absence of random heat fluxes [16]. The weight function $\omega(r_{ij})$ decreases monotonically with the particle–particle separation distance and becomes zero beyond the cutoff radius. $\zeta_{ij}^e$ is a random number with zero mean and unit variance. Each pair has an antisymmetric value of $\zeta_{ij}^e$ and $\zeta_{ij}^e = -\zeta_{ji}^e$ to ensure the energy of the interacting pair of particles is conserved. $\kappa_{ij}$ and $\alpha_{ij}$ are the strengths of the conductive and random heat fluxes. These coefficients are related and satisfy the following equation introduced by Ripoll [17]:

$$\kappa_{ij} = k_o k_B T_{eq}^2 \left(\frac{\epsilon_i + \epsilon_j}{2k_B T_{eq}}\right)^{n_\kappa} \tag{5}$$

$$\alpha_{ij} = \sqrt{2k_B\kappa_{ij}} \tag{6}$$

where $\epsilon = C_v T$ and $k_o$ is a constant having positive value that determines the thermal conductivity of DPD particles. $T_{eq}$ is the equilibrium temperature of the system and $n_\kappa$ is a constant which can be freely chosen. $n_\kappa$ is selected to be 2 in this study as is common in the previous DPDe studies [20,21,23,24]. For all the simulations, the dimensionless heat capacity, $C_v/k_B$, and $k_o$ were chosen to be $1.0 \times 10^5$ and $1.26 \times 10^{-4}$, respectively. These are the same values used in the benchmark simulations of one-dimensional unsteady heat conduction problems performed in our previous study [22] which were compared with the analytical and other DPDe studies.

### 2.2. DPD application for diffusive-ballistic heat transport

For the DPDe simulation of the diffusive-ballistic heat transport in thin films, the solution domain is set to be a two-dimensional lattice with $L$ and $N$ cells in $x$- and $y$-directions, respectively, as seen in Fig. 1. A cell is a square having a unit length, $a$. DPD particles are distributed uniformly in this domain and enclosed within the walls in extra layers outside of the domain having the constant temperatures $T_H$ and $T_C$ at the top and bottom of the walls, respectively. The number of wall layers was adjusted based on the cutoff radius of particle energy interaction. A periodic boundary condition was imposed in the $x$-direction, such that the simulations were considered to be one-dimensional. The initial temperature of the DPD particles for the simulations was set to be 1.0, and $T_H$ and $T_C$ were chosen to be 1.1 and 0.9, respectively, in DPD units.

The following section presents a detailed method that incorporates the effects of phonon mean free path into the DPD system by relating the length to the cutoff radius of energy interaction.

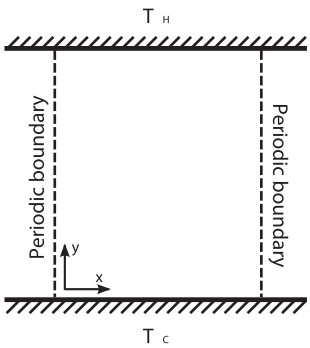


**Fig. 1.** Schematic of the boundary conditions of 1D heat conduction simulations.